

## ***Interactive comment on “Simulation of semi-explicit mechanisms of SOA formation from glyoxal in a 3-D model” by C. Knote et al.***

### **Anonymous Referee #3**

Received and published: 16 January 2014

Knote et al. implemented a number of SOA formation pathways from glyoxal into a regional model, used the model to simulate SOA formation over California, and compared model results to measurements during CARES/CalNex. They showed that the glyoxal SOA simulated by the various proposed production pathways can differ by a factor of 10. Key uncertainties include whether glyoxal SOA formation is surface-based or volume-based, whether it is reversible, and whether it is dependent on aerosol state

My initial response to the title of this paper was enthusiasm, as a thorough comparison between the different proposed pathways of glyoxal SOA formation and a comparison with high-temporal resolution measurements would be an important contribution to the current glyoxal-SOA debate. Unfortunately, the paper turn out to be much less informative. The most that can be drawn from the paper is that the glyoxal SOA simulated

C11141

using the current proposed pathways differ by as much as a factor of ten. Well, if indeed the differences are that large between the pathways, surely the AMS measurements can tell us something about which one(s) are way out of the ball park? But this kind of information was not given in the paper. I recommend major revision to the paper before publication.

Major comments:

1. The implementation of different glyoxal-SOA formation pathways into the model is a major undertaking. However, the ways these pathways were implemented was confusing. I realize that some of these pathways have only been demonstrated qualitatively, such that key parameters are not available or highly uncertain. However, even the parameterization of the SIMPLE pathway contradicts lab results. For example (Page 26712, lines 7-8) the authors stated: "There is no experimental evidence so far to determine whether this surface uptake can also take place on aerosols of any phase state, or whether a liquid phase is necessary". This is not true, c.f. Liggio et al. (2005) (JGR, 110D11, ). (I think the glyoxal-SOA formation in Stavrakou et al. (2009) and Fu et al. (2008) both take place only on wet aerosols and on cloud droplets.) Here the authors applied SIMPLE glyoxal surface uptake to the dry aerosol surface, and not at all to cloud droplet surface.

2. There is no actual "validation" or "comparison" of model results against measurements. The comparisons between model and measurements were limited to meteorological fields, precursors concentrations, and a few aerosol parameters (e.g. other aerosol species). There is only one figure that compares the "BASE" OA simulation against measured OA. I am surprised that the authors did not show the OOA concentrations from the AMS and the glyoxal SOA simulated for comparison. How do the glyoxal SOA predicted by different pathways improve the simulated correlation with OOA and SO<sub>4</sub>? These analyses might be more helpful in validating the different pathways.

The authors compared the measured and simulated glyoxal concentrations and stated

C11142

that the SIMPLE parameterization overestimated the removal due to SOA formation. I would argue that, given the uncertainty in the photochemistry of glyoxal and its precursors, the differences between the glyoxal concentrations simulated by different pathways shown here are trivial.

Minor comments:

1. Page 15, lines 20-22: "All cases except SIMPLE..., and in those no glyoxal SOA...": This sentence is confusing - please consider revising.
2. Page 26703, line 20: "There is no previous study on glyoxal-SOA formation in a 3-D regional model.": a missing reference is Li et al. (2013), *Atmospheric Environment*, 76, 200-207, doi: 10.1016/j.atmosenv.2012.12.005
3. Page 26725, lines 8-10: "The surface uptake coefficient finally was derived ...": The SIMPLE parameterization was not based only on mass-imbalance calculations, c.f. Liggio et al. (2005).
4. Some of the text in the figures are too small and illegible, e.g. Fig. 10, 12, and 13. Please consider revising.

---

Interactive comment on *Atmos. Chem. Phys. Discuss.*, 13, 26699, 2013.

C11143